GTOL
Version 7.2e [June 1, 2007]

Author: Thomas W. Burrows
Dept. of Energy Sciences and Technology
National Nuclear Data Center
Bldg. 197D
Brookhaven National Laboratory
P.O. Box 5000
Upton, NY 11973-5000
Phone: 631-344-5084 FAX: 631-344-2806
Email: nndctb@bnl.gov

Original Authors: **W.B. Ewbank**, Nuclear Data Project, Oak Ridge National Laboratory
B.J. Barton, National Nuclear Data Center, Brookhaven National Laboratory
L.P. Ekström and P. Andersson, Department of Nuclear Physics, Lund University

In this program, gamma-ray energies are used to derive a set of least-squares adjusted level energies. The net feeding at each level is calculated from the input gamma intensities and conversion coefficients. Unplaced or questionable gammas or gammas whose final level is ambiguous or unknown are ignored. The program parses the DSID of each data set and, if there is no indication of possible gamma records within the data set, skips it. In addition, the program will not calculate the intensity balancing for adopted data sets.

Input file:

(Sample input file: gtol.inp)

An ENSDF formatted file with the following optional information:

An option record with 'OPTION' in columns 1-6 may precede any dataset and contain any of the following options in free format.

Option	Meaning
NOREC	No recoil correction, *i.e.*, recoil correction has already been applied to Eγ
RECOIL	Perform recoil correction (DEFAULT)
MARKED	Process only datasets preceded by a card with "*GTOL" in columns 1-5
ALL	Process all datasets (DEFAULT)
DEG=	For the current data set, override default assumption of 1 keV where no uncertainty on the gamma energy is given. Following the equal sign may be either a number or a number followed by a percent sign ("%"). A number alone indicates the uncertainty on EG in keV while a number followed by a percent sign indicates the fractional percent uncertainty to be assigned.
DRI=	For the current dataset, assume a default uncertainty for the relative photon intensity when none is given. A number alone indicates the uncertainty on RI in the current relative units while a number followed by a percent sign indicates the fractional percent uncertainty to be assigned.

DTI= For the current dataset, assume a default uncertainty for the total transition intensity when none given. A number alone indicates the uncertainty on TI in the current relative units while a number followed by a percent sign ("%") indicates the fractional percent uncertainty to be assigned.

Note that an option card resets the defaults.

A level energy can be held fixed by adding the letters "F" or "G" somewhere in the energy field (columns 10-21). If "G" is used, the uncertainty of the fixed level energy will be added in quadrature with that derived from the least-squares adjustment. If the output option to create a new file containing the adjusted level energies is chosen, the "F" will be removed and a level documentation record will be added (`LEVEL ENERGY HELD FIXED IN LEAST-SQUARES ADJUSTMENT`).

If DRI or DTI are specified on an OPTION record, the assumed uncertainty may be overridden for an individual intensity, by adding an "E" separated from the intensity in either the RI or TI fields.

If DEG, DRI, or DTI are specified on an OPTION record and a new file is created, FOOTNOTE COMMENTS will be generated and inserted as necessary.

Output files:

1. Report file. The report file will contain a summary of the data input and actions taken by the program (*e.g.*, unplaced or questionable gammas ignored) and the following optional outputs for each data set:
   a. Comparison of input gamma energies to those calculated based on the adjusted level energies.
   b. Comparison of the input level energies to the adjusted level energies
   c. Comparison of calculated net feedings to each level with values input on B, E, or A records. Note: if the calculated net feeding overlaps zero within three standard deviations, the program will calculate estimated upper limits (90% confidence level) using two methods suggested by Louis Lyons in Statistics for nuclear and particle physicists (Cambridge University Press) and report these estimates if they differ by more than 0.01. The two methods are:
      i (Integral of gdB from 0 to Bl)/(Integral of gdB from 0 to infinity)=0.9 where g is the normal (Gaussian) distribution.
      ii Bl<Bm+1.28sigma.

   Sample output file: gtol.rpt
2. New file containing the adjusted level energies (Optional). Sample output file: gtol.out

Terminal dialog:

The program will request the input (default: gtol.inp) and report (default: gtol.rpt) file names and ask if you wish a new file created (default: No) and for the new file name, to suppress the gamma-energy comparison (default: No suppression), and to suppress the intensity comparison (default: No suppression). If the intensity comparison is not suppressed, there will be an additional

query asking for the uncertainty to be assumed for the theoretical uncertainty on the total conversion intensity. The choices are:

1) HSICC (Default): 3% uncertainty
2) BrIcc: 1.4%
3) Other: Give the percent uncertainty to assume

The progress of the program will be noted on the terminal as well as possible problems.

Command line mode:

The program may also invoked *via* the command line by entering gtol followed by a string with a leading per cent sign ("%") and the input parameters in the same order as in the terminal dialog separated by "%". A blank (" ") or "#" specifies that the program default be used. For output files, "null" (case insensitive) will direct the output to the null device (/dev/null under Linux). A simple example is:

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gtol <ENSDF filename>
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This will process in the specified ENSDF file with the program defaults.

Compilation and loading instructions:

This program requires subroutines from the NSDFLIB95 package.

Additional documentation:

B.J. Barton and J.K. Tuli. PHYSICS ANALYSIS PROGRAMS FOR NUCLEAR STRUCTURE EVALUATION. Brookhaven National Laboratory Informal Report BNL-NCS-23375/R (1977).
L.P. Ekström and P. Andersson. FORTRAN 77 VERSIONS OF STRING HANDLING SUBPROGRAMS AND THE PROGRAMS GTOL AND MEDLIST. Nuclear Physics Report LUNFD/(NFFR-3049)/1-27 (Lund University, Lund Sweden. 1983).

Version History:

Version	Date	Comments
5(0)	August, 1983	FORTRAN77 Version August 1983, LPE, Lund, Sweden. Based on VERSION 4(15) as of 6-Jan-82. MAIN CHANGES: 1) FORTRAN 77 using STR77 Library. 2) Number of levels, gammas, fixed levels as parameters. 3) Some unused options removed. 4) Some options added.

5(1)	February, 1986	MAIN CHANGES: 1) Localized program to improve paging rate on TOPS-10. 2) Changed terminal dialog. 3) Size of output reduced. 4) Option to create a new file with calculated level energies included. 5) Check of GAMMA continuation record for final level (FL=) formalism and other quantities, which may affect the calculations. 6) Ignores data sets whose DSID's indicate that there are no gammas present. KNOWN PROBLEMS (Common to all versions): 1) Field width overflows when there are very precise gamma energies. 2) Matrix inversion sometimes unstable when there is only one transition to or one transition from a level.
5(2)	June, 1986	MAJOR CHANGES: 1) Converted from Swedish STR77 library to NNDC F77STR and NSDCNV libraries
5(3)	August 8, 1986	Add VAX MDC
5(4)	December 11, 1986	Add IbmPC MDC
5(5)	September 4, 1987	1) Corrected logic causing floating-point overflow in subroutine MINV. 2) Corrected minor parsing problems in subroutine GA2DEC. Also rewrote this subroutine to reduce redundant coding using modules from RADLST and the new subroutines CHNGS1 and CHNGS2. 3) Corrected field-width overflow problems by increasing associated string lengths and format statements from 8 to 10 (Maximum size of energy fields in ENSDF). Since this increased the size of the output, added checks to not list blank lines when there are no old gamma energies to be compared to. 4) Removed output of "F" for level energies. 5) Brought modules associated with these corrections more up to current F77 standards and philosophy.
5(6)	November 2, 1987	VAX MDC OPEN READONLY added for input dataset file

5(7)	August 30, 1989	1) Added checks for a. Number of levels exceeding number of gammas plus fixed levels b. Matrix being singular In both of these cases it will list connected but not fixed levels which either have a. No gammas feeding them b. No gammas de-exciting them since this seems to be the most common cause of the problem 2) General cleanup of code 3) Added logic to reduce extraneous calculations and output 4) Restored lost coding to remove output of "F" for level energies and to output a "DL" record for these levels 5) 5) Automatic suppression of intensity comparison for ADOPTED LEVELS, GAMMAS dataset
5(8)	September 12, 1989	1) Corrected logic error which caused (G,G') datasets to be rejected 2) Changed string lengths and output formats for I/O files to reduce changes of truncation
5(9)	June 12, 1990	Changed statement order (CHKALF), F format spec (INTOUT) *etc.*, for PC FORTRAN
5(10)	July 24, 1990	Corrected error in INTOUT which gave log of a negative number
5(11)	December 13, 1990	1) Corrected error in INTOUT which gave log of zero 2) Delinted using F-LINT 2.71
5(12)	October 15, 1992	Added Machine coding for ANS

6.0	April 7, 1993	Merged IBM PC test version of 28-Feb-91 01 with distributed version 5(12) [15-Oct-92]. IBM PC changes were: 1) Reworked internal storage to fit into limitations of real mode of MS/DOS. a. Most argument passing to subprograms replace by COMMON's. b. Replaced WAA(NLE,NLE) by WAA(NSTORE) with NSTORE=(NLE*NLE+NLE+1)/2 and added bookkeeping function STRLOC 2) Replaced general-purpose matrix inversion routine MATINV and MINV by a new MATINV which uses a specific algorithm for symmetric matrices. 3) Added PCTIME and PCDATE routines for IBM PC which access the MS FORTRAN routines GETTIM and GETDATE As a result of 1b) and 2) the code runs slower. However, for NLE=300 memory requirements were reduced by about 658k. Other changes: 1) Added overlay module indicators for use in separating source code for compilation and linking on IBM PC 2) Added check on diagonal matrix elements after inversion - If any negative values, no least-squares adjustment 3) Added check on E(level) after matrix multiplication - If any negative values, level processing terminated 4) Removed redundant output of fixed levels list 5) Replaced numeric comparison for FL= with string comparison and corrected minor logic errors 6) Added bookkeeping on how the level was fixed 7) Always assume that the first level is fixed 8) Added logic for non-numeric levels 9) Update FL= when new file option specified 10) Warn about levels being out of order in new output 11) Increased NFIX=NLE/2 to NFIX=NLE 12) Reduced verbosity of report by only putting out relevant input data (should also reduce elapsed time due to I/O) 13) Corrected output field width overflow in intensities 14) Kept non-numeric uncertainties on feeding radiations 15) Hold levels of the form S_p+x or S_n+x fixed and ignore de-exciting gammas 16) Correction of minor logic errors in calculating total intensities 17) If NB not given, assume 1.0/BR in agreement with other codes 18) Account for 3% uncertainty in CC theory when calculating TI
6.1	July 12, 1993	Corrected error in calculating net g.s. feeding (100*BR+TNRF to 100+ TNRF)

6.2	November 26, 1993	1) Removed error introduced in version 6.1. 2) Ignore gammas with non-numeric EG. 3) Implemented Asilomar F and P recommendations to allow specifications of DEG, DRI, and DTI when not given. 4) For DEG, DRI, or DTI of "AP", uncertainty set to three times that for field. 5) If "&", in column 77, RI=DRI=(RI+DRI)/2 and TI=DTI=(TI+DTI)/2 assumed. 6) If "LT" or "LE" in DRI or DTI field, RI=DRI=RI/2 or TI=DTI=TI/2 assumed. 7) Automatically remove previous GTOL-generated "DL E" records.
6.2a	April 9, 1999	1) Y2K compliance 2) Increased ANSI FORTRAN 77 compliance 3) Check for and skip Ionized Atom 4) Properly recognize H record
6.3	May 23, 2000	1) Implemented logic for FL=? 2) Added estimates of upper limits of the calculated net feeding using the methods of Lyon 3) Corrected bug in subroutine CHGCRD 4) Removed overlay logic
6.3a	January 8, 2001	Corrected logic errors in replacing "FL="'s
6.4	March 1, 2001	Added UNX MDC coding. (RRK)
6.4a	July 11, 2001	Corrected output overflows when adding new Comment record for DEG, *etc.*
6.4b	December 3, 2003	1) Increased NLE from 300 to 1000 and NGA from 3*NLE to 4*NLE. 2) Left justify new level energies in output file. 3) Corrected output overflow problem in RADDEC. 4) Corrected string range problem in IDDEC.
7.0	February 18, 2004	1) Converted to Fortran 95 2) Command line input added
7.1	October 6, 2005	1) Incorporated PNPI F77 versions 6.4c and 6.4d a. Additional output after matrix inversion comparing the level energies and transition energies including χ^2. These were moved to separate subroutines and are only output if matrix inversion is successful b. Converted to double precision 2) Added check against Chi**2 (critical) and output warning to terminal and report file if deviant

7.1a	October 17, 2005	1) Corrected problem in comparing transition energies when gamma could not be placed within +-10 keV 2) Added summary of gammas which could not be placed within +-10 keV to terminal output
7.2	November 14, 2005	1) Changed logic for processing FL=? so that RI and TI would be included in RI(OUT) and TI(OUT) 2) Added query to allow user to specify theoretical DCC to be assumed (HSICC, BrIcc, or Other) 3) Attempted to check metastable state continuation records to see if there is no IT decay. If so, GTOL assumes level is fixed and adds the uncertainty of the state in quadrature with that derived from the least-squares adjustment 4) Added option to place "G" in level energy field. Similar to "F" option but uncertainty will be added in quadrature with that derived from the least-squares adjustment 5) Added check for two gammas from same parent to same daughter 6) Attempted to make the level and transition energy tables more readable 7) If Chi**2 (critical) test fails, give a short summary of the most discrepant gammas. 8) Corrected logic errors in converting ranges to values and uncertainties for GAMMA continuation records 9) Corrected some field width overflow problems in intensity comparison 10) Restored ANS MDC for opening output files
7.2a	November 17, 2005	Corrected conflict in type for dummy real variable in calls to RLSCN in subroutine READIN
7.2b	January 20, 2006	1) Corrected formula for chi**2 critical for N>30 2) Output to report degrees of freedom if chi**2 test fails 3) Some cleanup of terminal output
7.2c	May 15, 2006	1. Reworked logic so matrix would be recalculated if "FL=" gamma had not been placed within +-10 keV 2. Used data created by Tibor Kibedi to extended critical Chi**2 DATA statement from 30 to 200 3. Added check when adjusting energies for fixed daughter level uncertainties so that fixed levels would not be adjusted

7.2d	November 1, 2006	1. Added check for existence of %IT when checking decay modes. If found, level will not be held fixed even if total of other modes is greater than 99.95%. Added checks for other types of decay (e.g., %N or %P) 2. Corrected bug apparently introduced in 7.2 when attempt was made to process FL=? so that RI and TI would be included in RI(OUT) and TI(OUT) 3. Corrected bug apparently introduced in 7.2 when the "G" option was introduced
7.2e	June 1, 2007	1. Added check on unrealistically large diagonal matrix elements to handle differences between LF95 and DVF 2. Added check for level energies such as "EN+X" and ignore deexciting gammas 3. Changed default ICC's from HSICC to BrIcc 4. Fixed spurious error message when End of File followed an END record

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